Electronic Materials and Photonics
Room 207 A W - Session EM2+AIML+AP+CPS+MS+SM-TuA

Advances in AI and Machine Learning within the Semiconducting Industry

Moderator: Erica Douglas, Sandia National Laboratories

4:00pm **EM2+AIML+AP+CPS+MS+SM-TuA-8 Improved Design-of-Experiments and Process Modeling with Generative AI***, Somilkumar Rathi, Muthiah Annamalai,* Panmo LLC

Small volume semiconductor, photonic and materials manufacturing largely uses One-Factor at-a time (OFAT) to discover process window instead Design of Experiments (DOE). We demonstrate, *Panmo Confab,* a Generative AI based DOE and process-flow-design platform to accelerate process window discovery. Large volume semiconductor, photonic and materials automation tools have relied on statistical process control (SPC), design of experiments (DOE) and yield modeling techniques which are fairly manual and depend on specialized tools and deep knowledge [1,2]when such tools are not used we get a sub-optimal outcomes for process development teams through using one-factor at a time (OFAT). In this article we report, and demonstrate, *Panmo Confab* a Generative AI based process flow tracking and design of experiments platform to accelerate flow designs and generating DOEs. Previously our tool was used without Generative AI, features to show improvement in process discovery for plasmonic nanocavity fabrication [4]. The unique innovation of our tool is to use the emerging technology of large language models (LLM), like BERT or ChatGPT [5,6] and science of causality [3] to enable generation of process flows with a description. Our tool is presented in both on-premises and Software-as-a-Service (SaaS) formats.

References:

1. Montgomery, D. C. Design and analysis of experiments. (John Wiley & sons, 2017).

2. May, G. S., & Spanos, C. J. Fundamentals of semiconductor manufacturing and process control. (John Wiley & Sons, 2006).

3. Pearl, Judea, and Dana Mackenzie. The book of why: the new science of cause and effect. (Basic books, 2018).

4. Annamalai, M., Rathi, S., Methodology for robust process window discovery in plasmonic nanostructures", Proc. SPIE 13111, Plasmonics: Design, Materials, Fabrication, Characterization, and Applications XXII, 131110A (2024).

4:15pm **EM2+AIML+AP+CPS+MS+SM-TuA-9 Foundation Models in Semiconductor R&D: A Study on Segment Anything***, Fei Zhou,* Sandisk Corporation

Quantitative analysis of scanning and tunneling electron images is crucial in semiconductor manufacturing, particularly for defect detection, process margin checking, and morphology quantification. Traditional AI/ML approaches, such as using recurrent neural networks, require large labeled datasets and extensive transfer learning to generalize across different imaging conditions. Developing a usable AI tool for proof-of-concept demonstrations demands significant engineering effort and GPU resources, making these methods costly and time-consuming. These challenges are especially pronounced in semiconductor R&D, where fast turnaround, high accuracy, and efficient use of engineering resources are essential.

The Segment Anything Model (SAM) introduces a novel training free segmentation approach, eliminating the need for task-specific retraining while providing robust and efficient segmentation across diverse semiconductor imaging requirements. This paper explores SAM's application in semiconductor image analysis, demonstrating its ability to segment complex nanoscale features without prior dataset exposure. We assess SAM's performance in automated defect detection, where challenges such as varying defect morphology, background noise, and process-induced variations exist. With appropriate prompting and post-processing techniques, SAM adapts to different imaging conditions, offering a rapid, low-cost, and high-accuracy solution.

Additionally, we examine SAM's limitations, particularly in scenarios where the region of interest is small and contains limited useful pixel data. By employing image enhancement techniques, we demonstrate how SAM can effectively segment defects even in low-information conditions. Furthermore, we explore how integrating grounding techniques with SAM can expedite segmentation post-processing, further improving efficiency in real-world applications.

Our case studies show that SAM significantly reduces resource overhead and enables semiconductor image analysis automation, achieving saving of >100 engineering hours and >20 GPU hours per project. Its foundation model architecture allows it to generalize across different defect types, backgrounds, and imaging techniques without additional data labeling or fine-tuning. These findings suggest that integrating SAM into semiconductor workflows enhances efficiency, lowers costs, and accelerates R&D decision-making by providing a scalable and cost-effective solution for high-precision image segmentation. This study highlights the transformative potential of foundation models in semiconductor engineering, paving the way for broader adoption of AI-driven automation across the industry.

4:30pm **EM2+AIML+AP+CPS+MS+SM-TuA-10 MOFCreatioNN: A Novel Modular Machine Learning Approach for Designing 'Undesignable' Metal-Organic Frameworks.** *, Satya Kokonda,* Charter School of Wilmington

Many critical material discovery processes remain too complex for traditional computational modeling, necessitating costly and time-intensive experimentation. Here, we present a generalizable, application-driven methodology for material design, demonstrated through a case study in photocatalysis. Using a reinforcement learning ensemble, we generated 120,000 novel metal-organic frameworks (MOFs) optimized for CO_2 heat of adsorption and CO_2/H_2O selectivity. A multi-objective fitness function—incorporating stability, catalytic potential, cost, sustainability, and adsorption properties—enabled computational modeling of photocatalytic performance aligned with industrial criteria. To enhance efficiency and prevent feature overfitting, a predictor funnel system iteratively filtered low-scoring candidates, narrowing the search space to 17,315 MOFs and improving computational efficiency by 313%. Our system, MOFCreatioNN, designed two high-performing, de novo MOFs: a Cr-based MOF with a photocatalyst score 239% higher than the control, and a Mn-based MOF that outperformed all baselines across every evaluated metric, demonstrating robustness against imperfect fitness functions. The proposed MOFs meet key synthesis and operational thresholds—including X-ray diffraction consistency with known structures, predicted synthesizability, temperature stability >300°F, and viable water stability—making them practical for real-world applications. Furthermore, we identify actionable design heuristics, such as the significant impact of the $N_2$62 metal cluster on photocatalytic performance. By integrating industrial considerations such as cost, stability, and environmental viability into the modeling process, this work showcases a scalable framework for the AI-driven design of industrially relevant materials in domains previously considered computationally intractable.

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